Supplementary Material (ESI) for New Journal of Chemistry

Supplementary Information

SYNTHESIS AND COMPLEXATION STUDY OF (1,4-LINKED)-HOMOTHIAISOCA LIXNAPHTHALENES

Table of Contents

^{1}H and ^{13}C NMR spectra of compounds **16a-d**: Pages: **S2-S5**

^{1}H and ^{13}C NMR spectra of compounds **12a-b** and **12c-d**: Pages: **S6-S7, S9, S11**

^{1}H and ^{13}C NMR spectra of compounds **17b** and **17c**: Pages: **S8** and **S10**

Chemical shift changes ($\Delta\delta$) for protons on **12a** vs added AgO_2CCF_3: Page **S12**

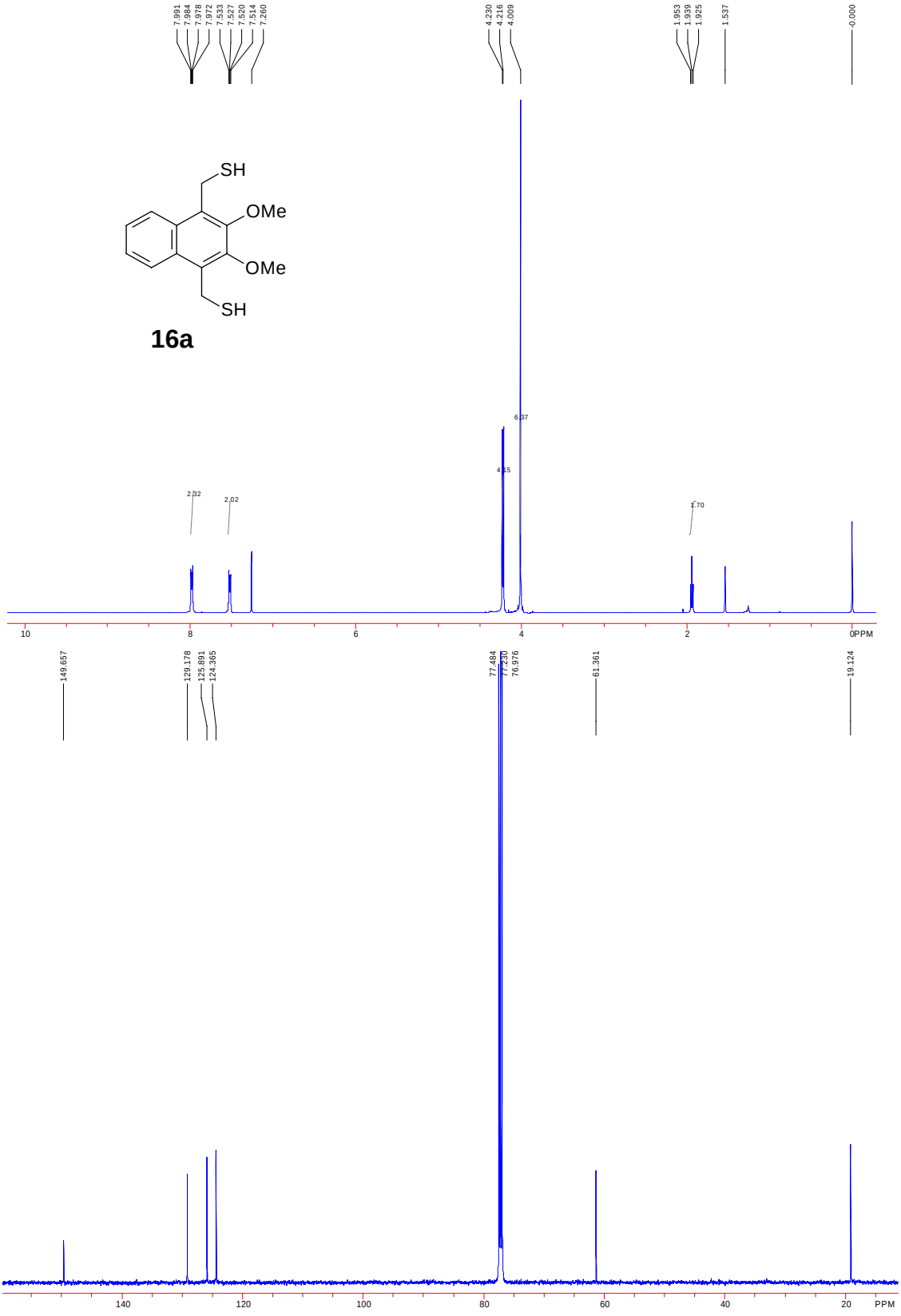
Chemical shift changes ($\Delta\delta$) for protons on **12b** vs added AgO_2CCF_3: Page **S13**

Chemical shift changes ($\Delta\delta$) for protons on **12a** vs added $HgCl_2$: Page **S14**

Chemical shift changes ($\Delta\delta$) for protons on **12b** vs added $HgCl_2$: Page **S14**

Non-linear Curve Fit Plots for **12a** and **12b** vs added AgO_2CCF_3: Page **S15**

Non-linear Curve Fit Plots for **12a** and **12b** vs added $HgCl_2$: Page **S16**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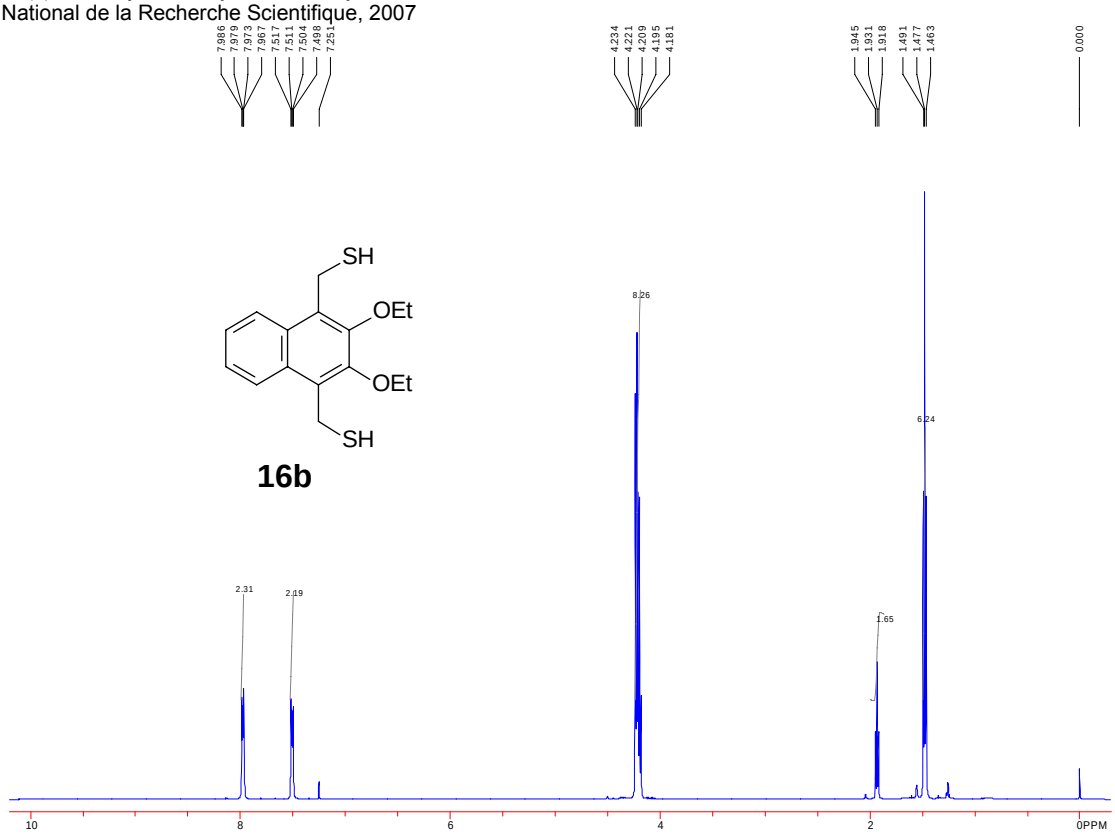
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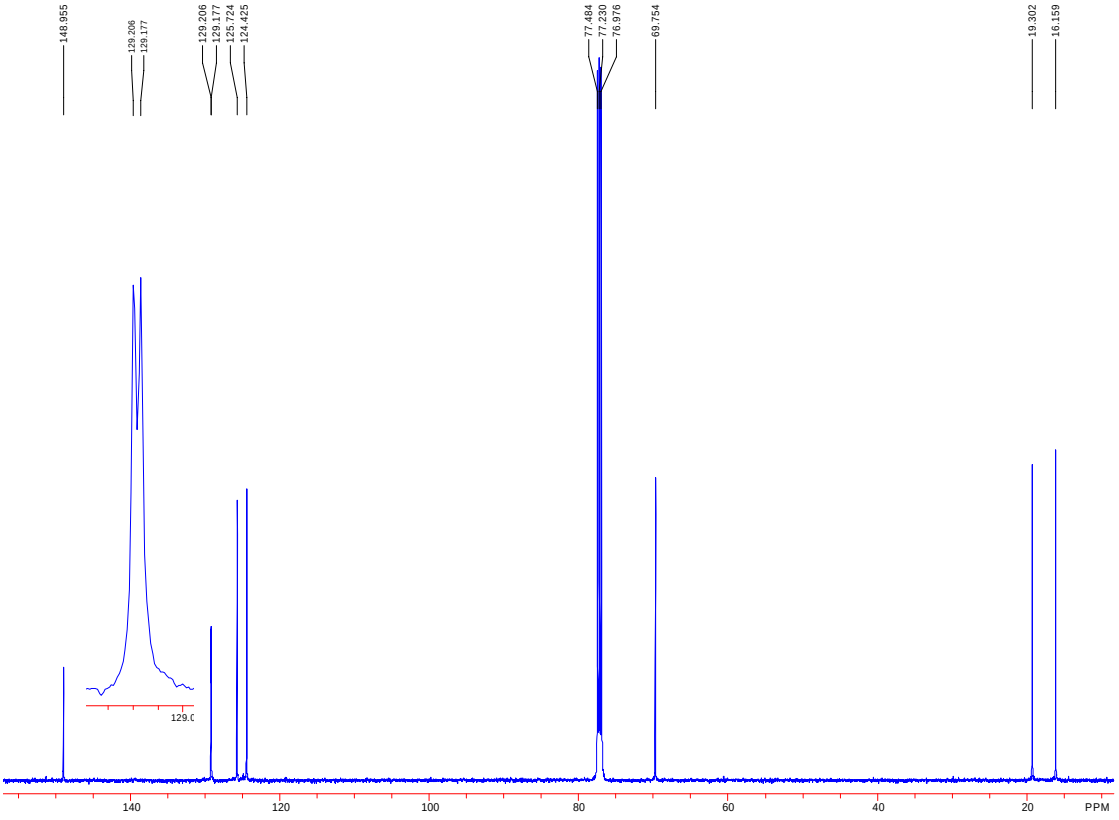
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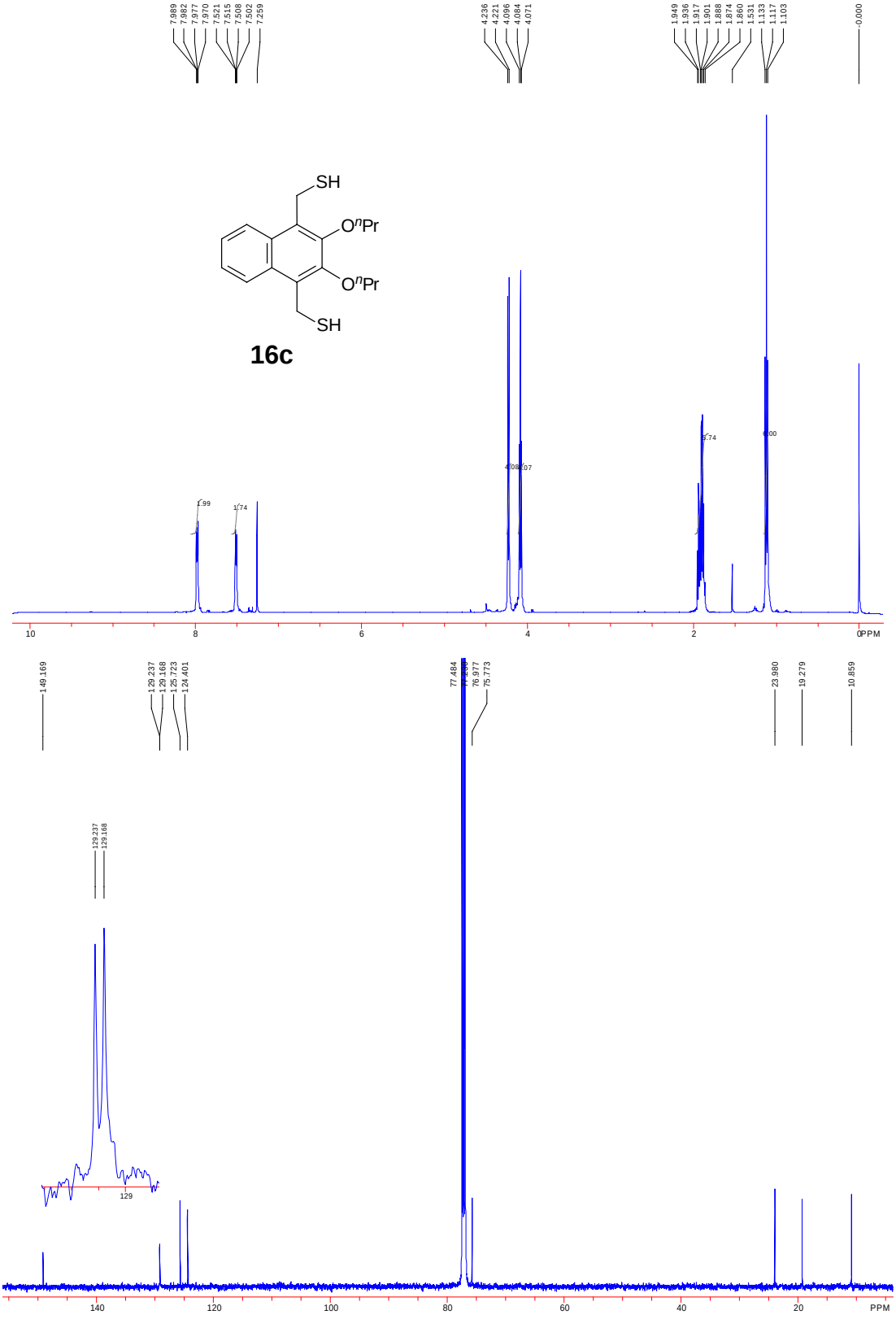
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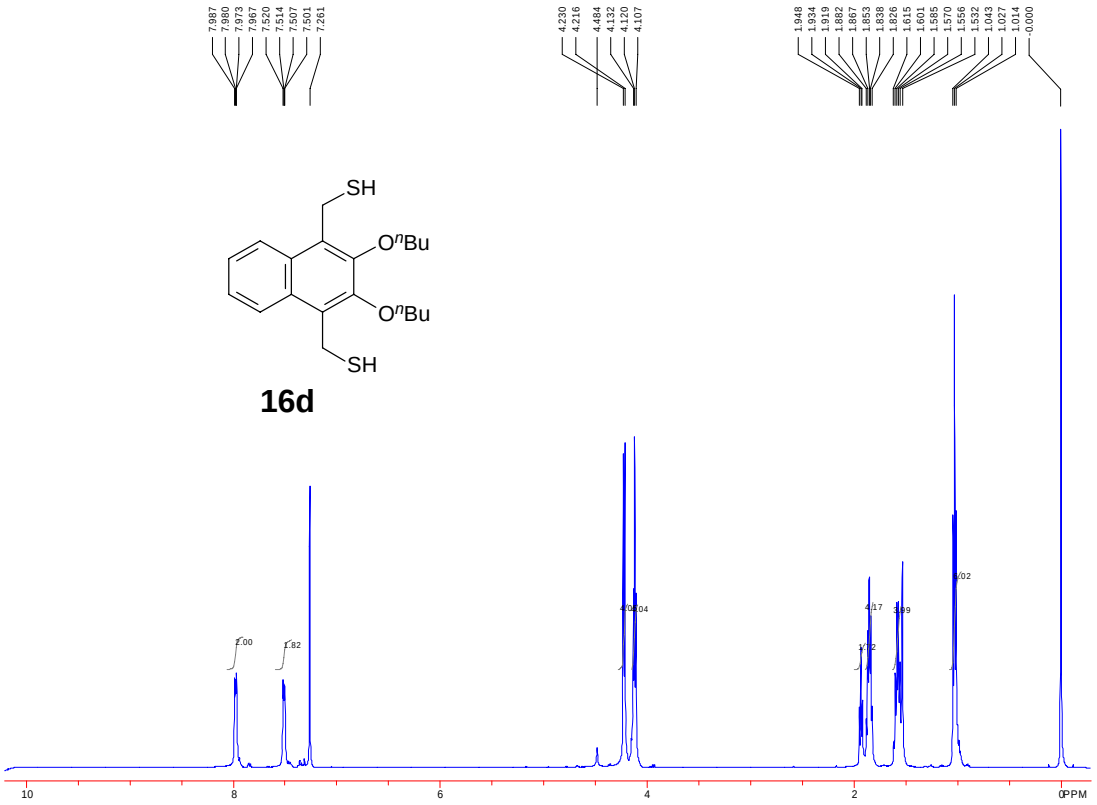
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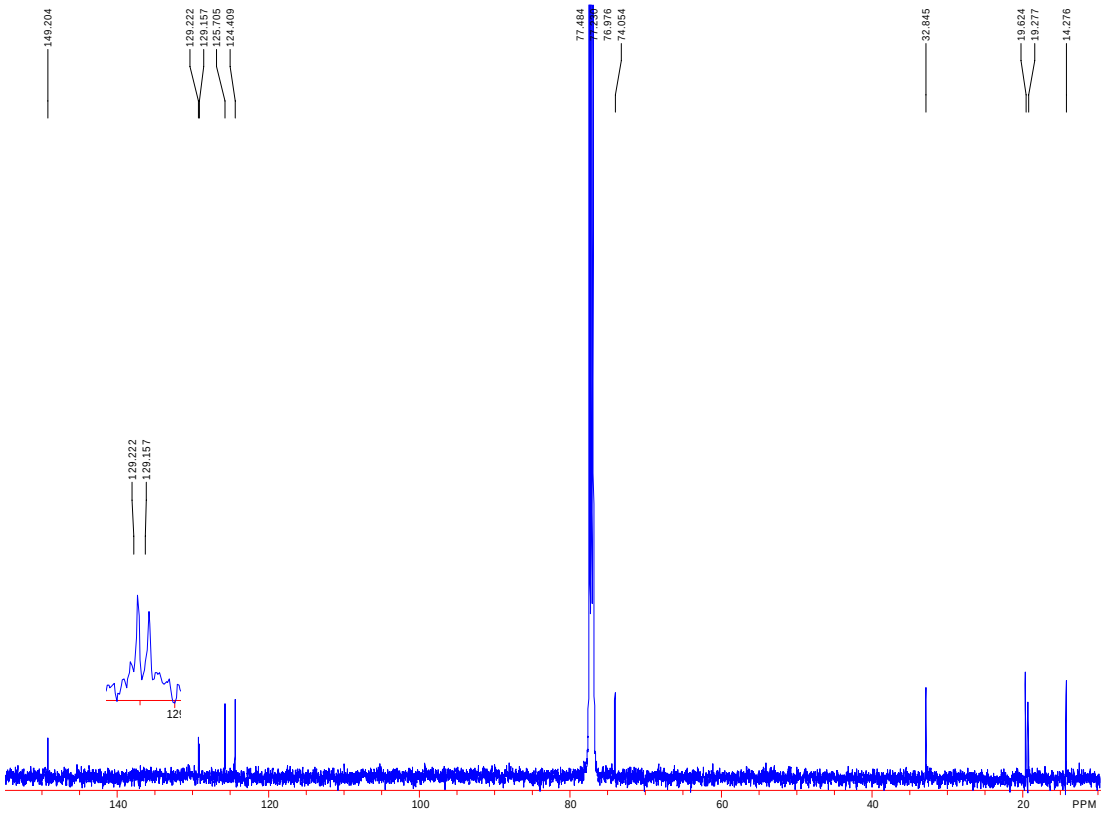
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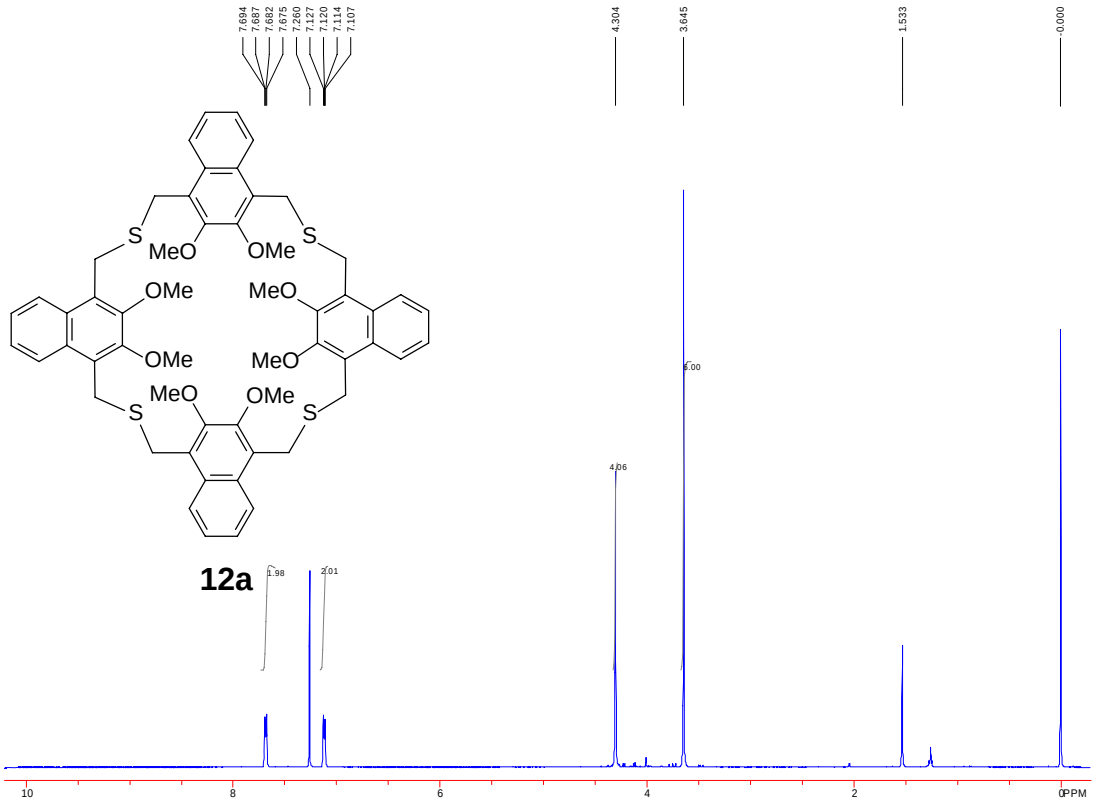
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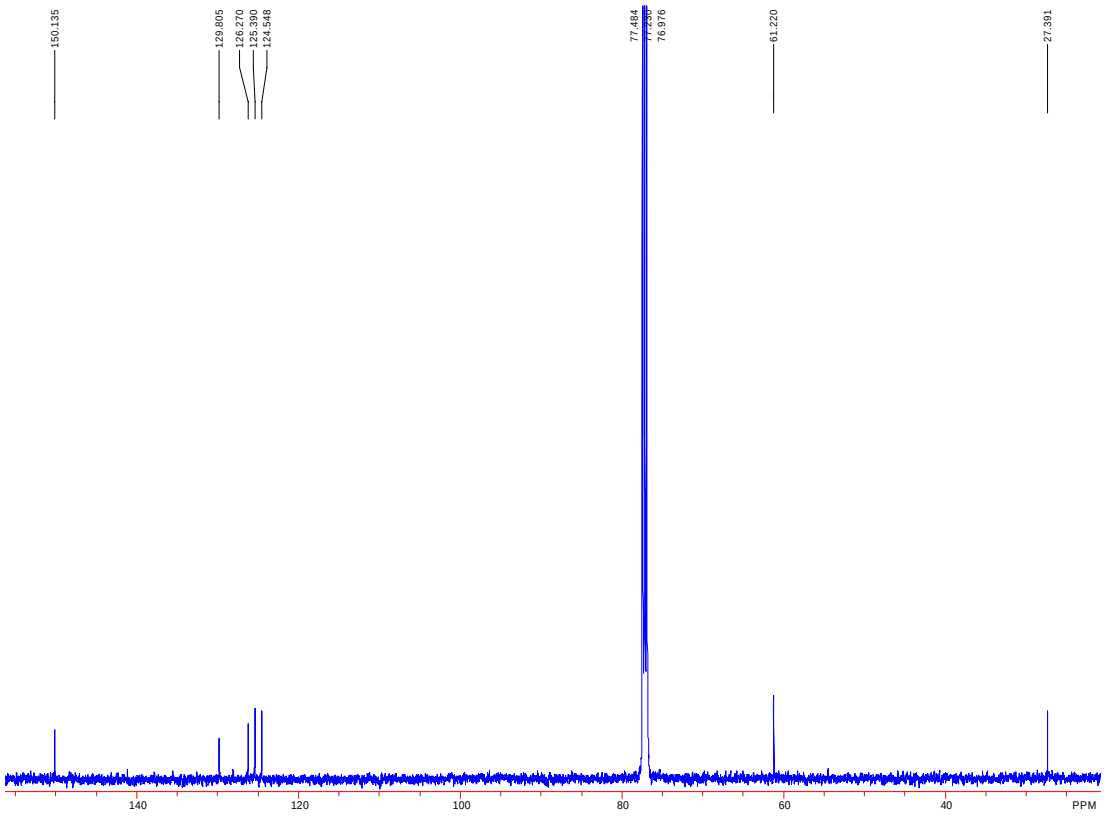
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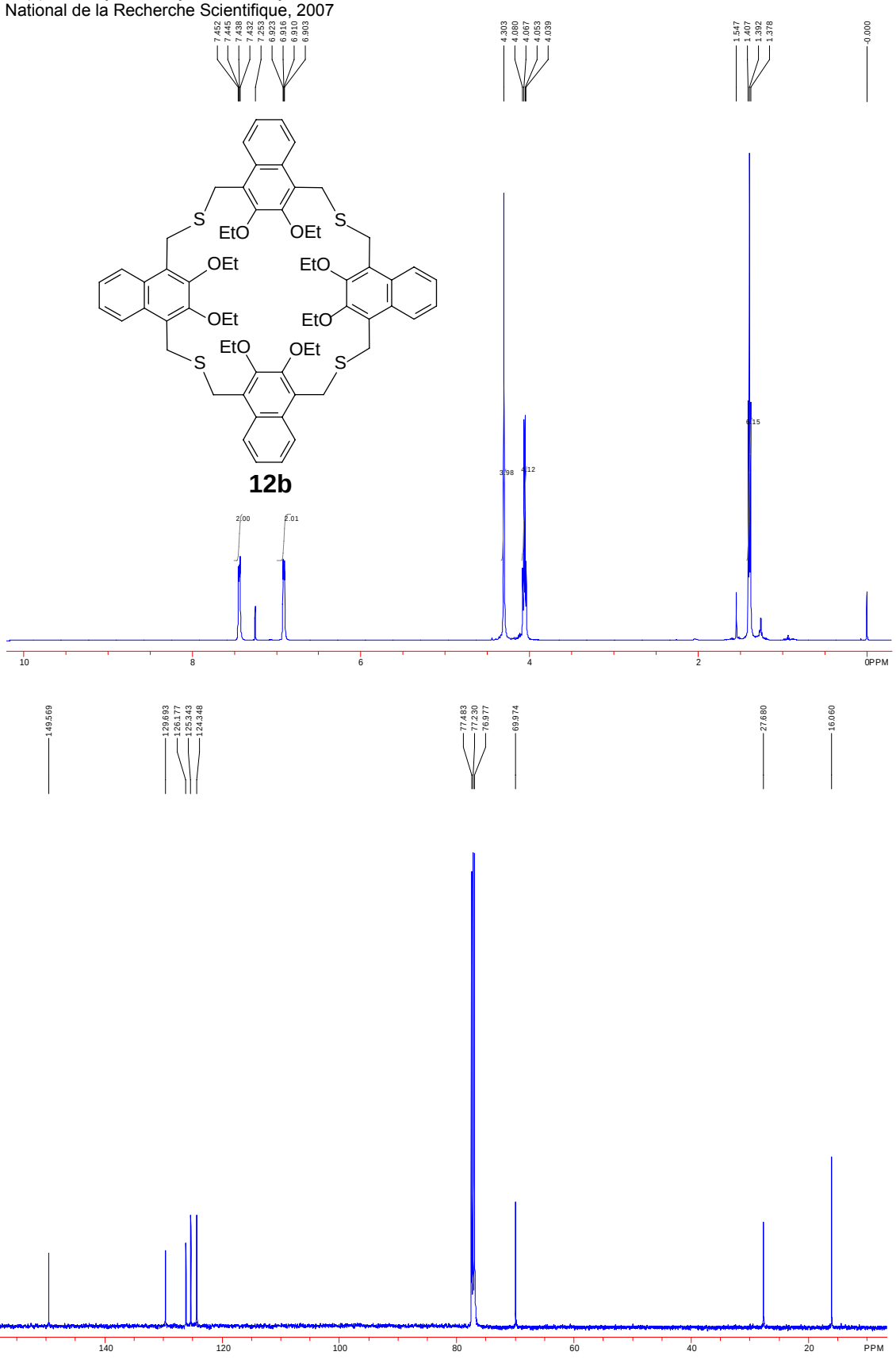
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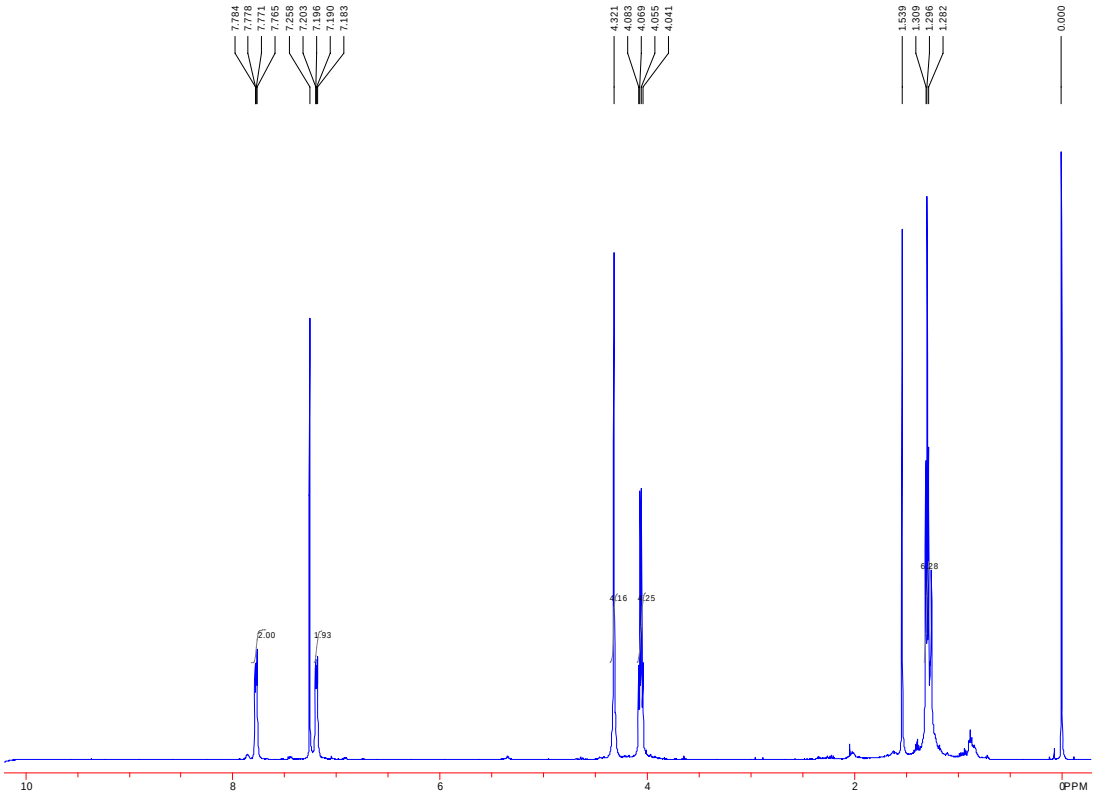
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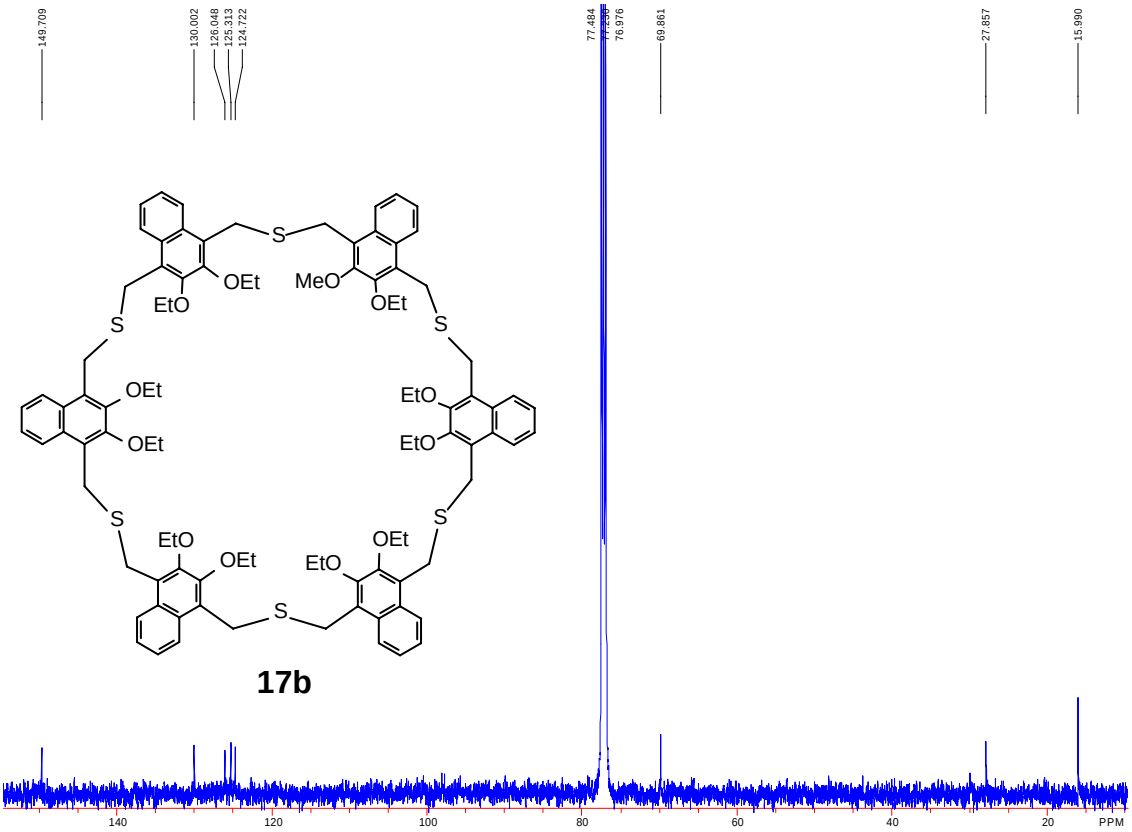
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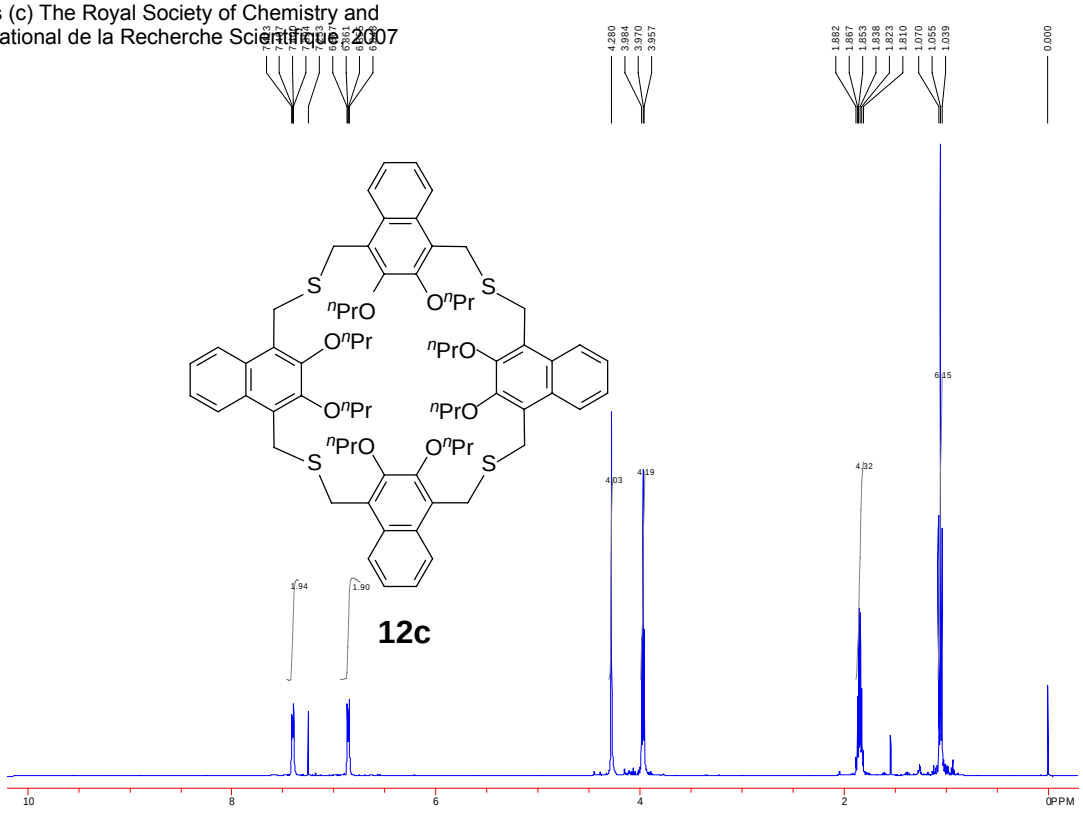
17b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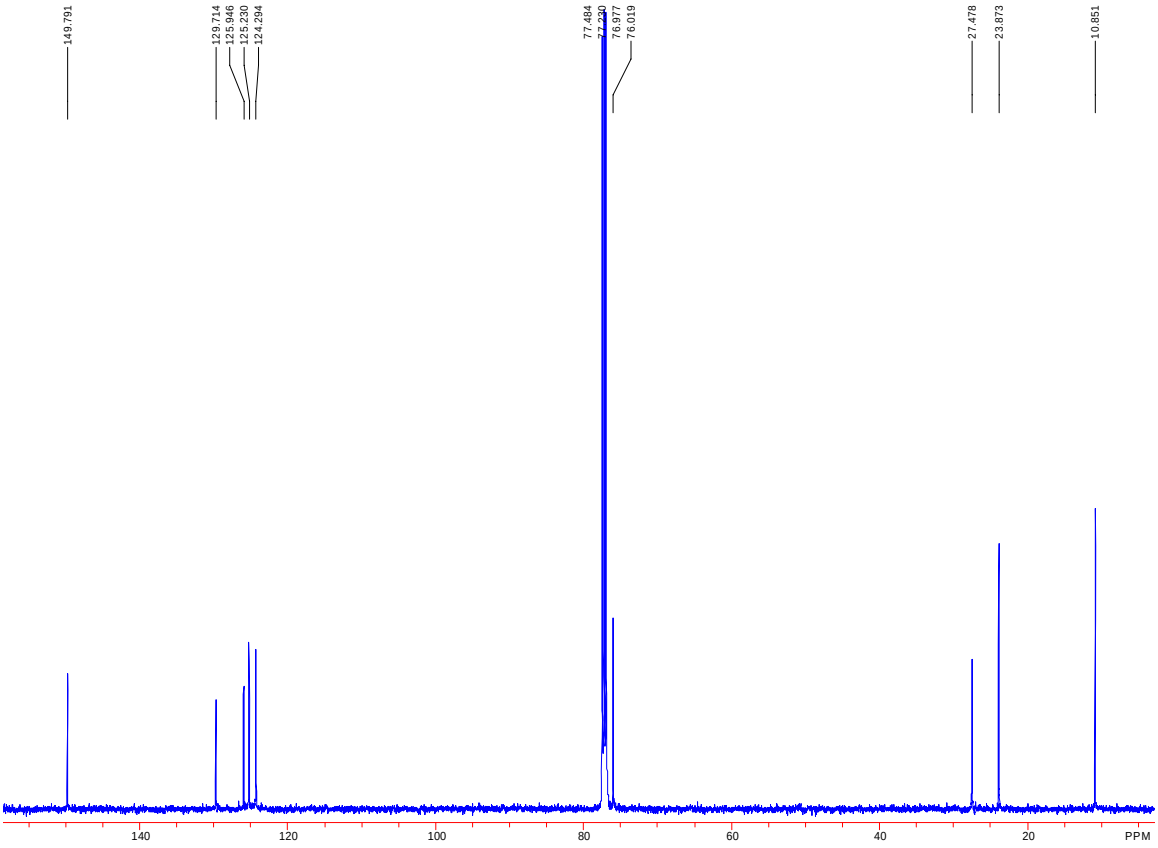
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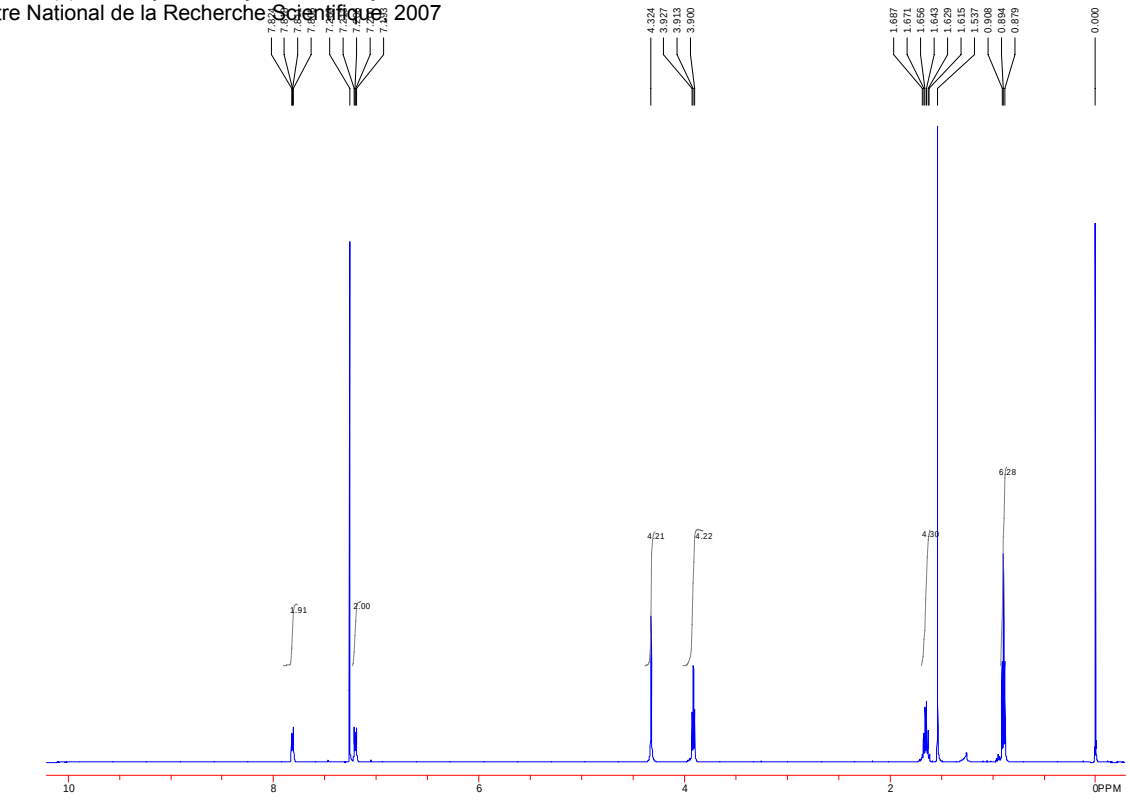
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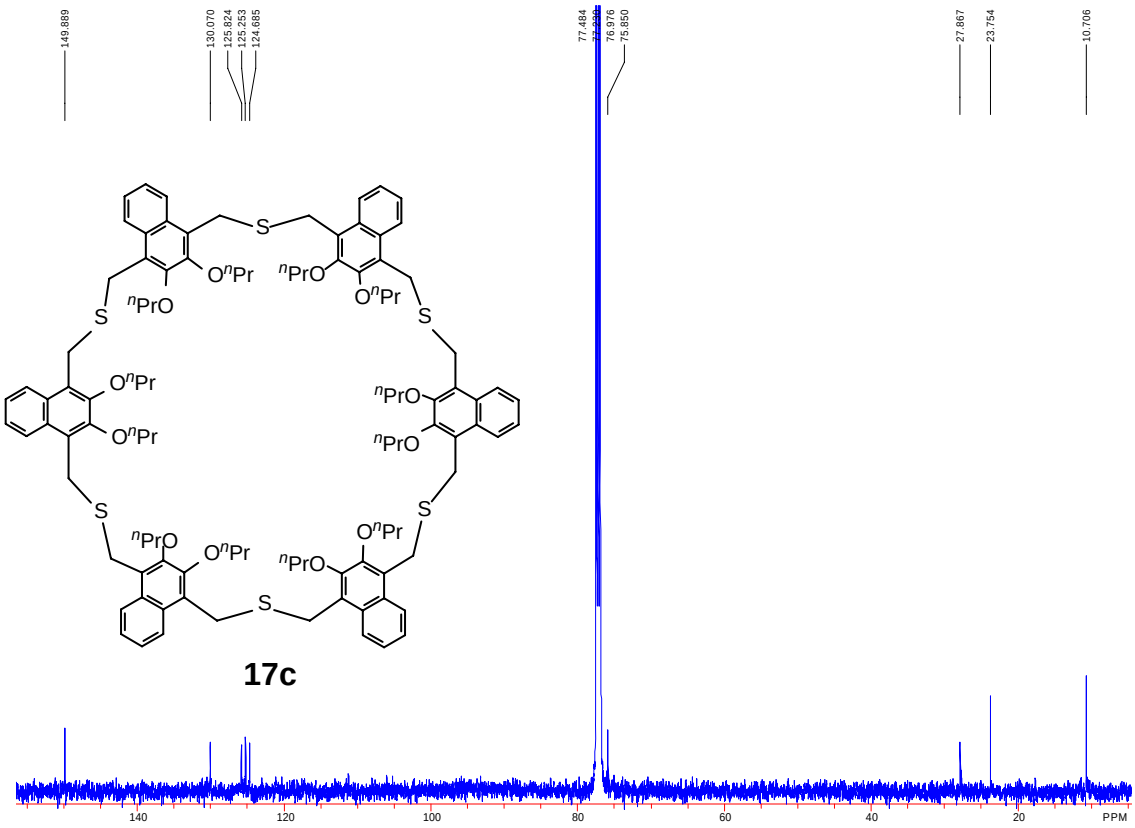
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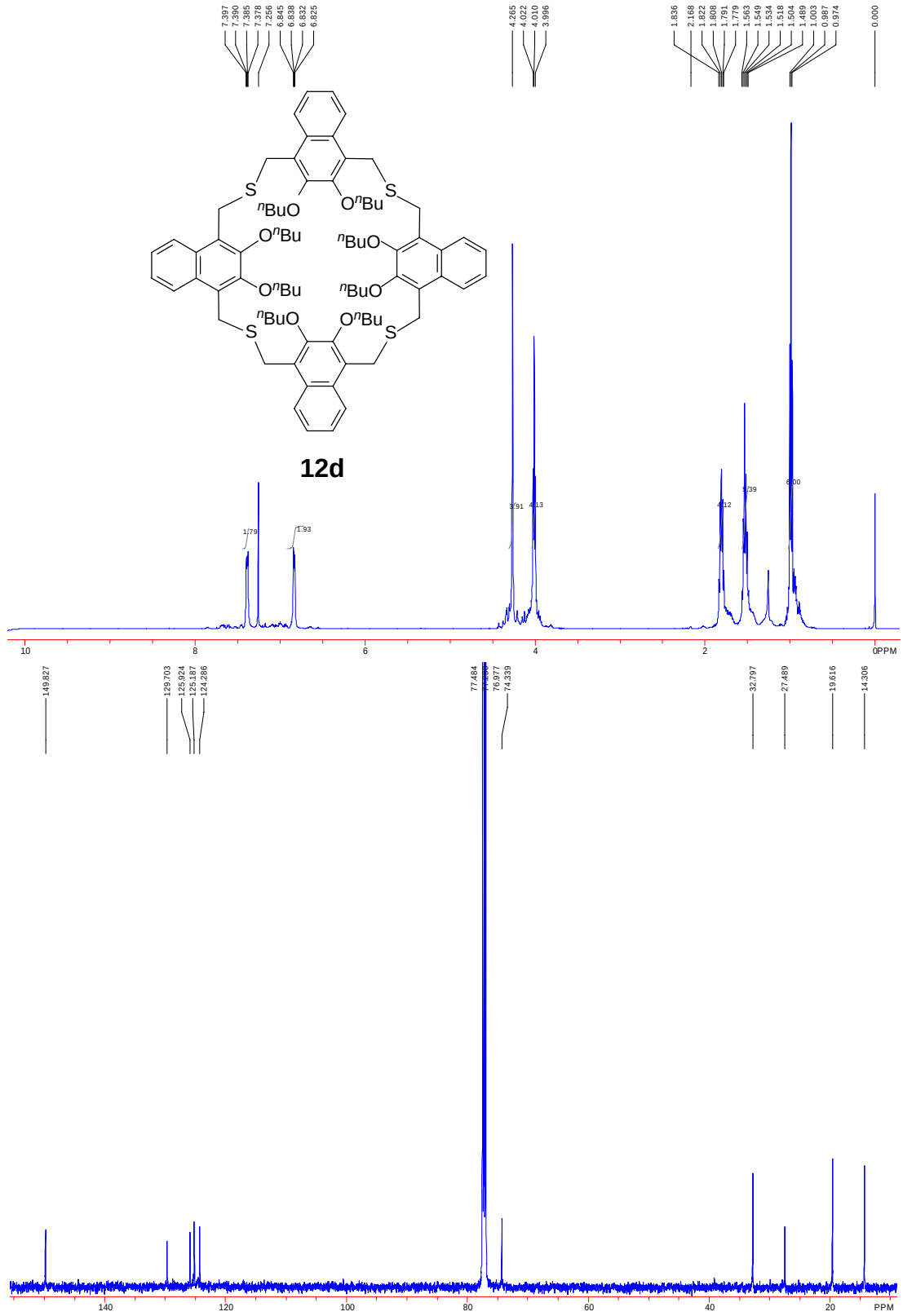
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Appendix 1 Chemical shift changes (Δδ) for protons on **12a** in 1:9 CD_3CN-$CDCl_3$ at 298 K *versus* added AgO_2CCF_3 solution (5.22×10^{-3} M) (Δδ are absolute values).

Run #1:

Entry	[Ag^+]	[12a]	[Ag^+]/[12a]	δ_{Ar} (ppm)	$\Delta\delta_{Ar}$ (ppm)	δ_{SCH_2} (ppm)	$\Delta\delta_{SCH_2}$ (ppm)	δ_{OCH_3} (ppm)	$\Delta\delta_{OCH_3}$ (ppm)
1	0.00	4.84×10^{-4}	0.00	**7.115**	0.000	**4.301**	0.000	3.666	0.000
2	2.48×10^{-4}	4.61×10^{-4}	0.54	7.121	0.005	4.339	0.038	3.699	0.033
3	3.26×10^{-4}	4.54×10^{-4}	0.72	7.120	0.005	4.351	0.050	3.707	0.041
4	4.01×10^{-4}	4.47×10^{-4}	0.90	7.124	0.008	4.361	0.060	3.713	0.047
5	4.74×10^{-4}	4.40×10^{-4}	1.08	7.124	0.009	4.370	0.069	3.717	0.051
6	6.47×10^{-4}	4.24×10^{-4}	1.53	7.124	0.009	4.390	0.089	3.728	0.062
7	8.08×10^{-4}	4.09×10^{-4}	1.97	7.126	0.010	4.406	0.105	3.738	0.072
8	9.58×10^{-4}	3.95×10^{-4}	2.42	not clear	-	4.418	0.117	3.745	0.079
9	1.10×10^{-3}	3.82×10^{-4}	2.87	not clear	-	4.428	0.127	3.751	0.085

Run #2:

Entry	[Ag^+]	[12a]	[Ag^+]/[12a]	δ_{Ar} (ppm)	$\Delta\delta_{Ar}$ (ppm)	δ_{SCH_2} (ppm)	$\Delta\delta_{SCH_2}$ (ppm)	δ_{OCH_3} (ppm)	$\Delta\delta_{OCH_3}$ (ppm)
1	0.00	4.84×10^{-4}	0.00	7.116	0.000	4.301	0.000	3.666	0.000
2	2.48×10^{-4}	4.61×10^{-4}	0.54	7.121	0.005	4.339	0.038	3.700	0.034
3	3.26×10^{-4}	4.54×10^{-4}	0.72	7.124	0.008	4.350	0.049	3.708	0.042
4	4.01×10^{-4}	4.47×10^{-4}	0.90	7.126	0.010	4.360	0.059	3.716	0.050
5	4.74×10^{-4}	4.40×10^{-4}	1.08	7.126	0.010	4.369	0.068	3.722	0.056
6	6.47×10^{-4}	4.24×10^{-4}	1.53	7.128	0.012	4.390	0.089	3.735	0.069
7	8.08×10^{-4}	4.09×10^{-4}	1.97	not clear	-	4.404	0.103	3.744	0.078
8	9.58×10^{-4}	3.95×10^{-4}	2.42	not clear	-	4.416	0.115	3.752	0.086
9	1.10×10^{-3}	3.82×10^{-4}	2.87	not clear	-	4.426	0.125	3.758	0.092

Appendix 2 Chemical shift changes (Δδ) for protons on **12b** in 1:9 CD_3CN-$CDCl_3$ at 298 K *versus* added AgO_2CCF_3 solution (5.07×10^{-3} M) (Δδ are absolute values).

Run #1:

Entry	$[Ag^+]$	[12b]	$[Ag^+]/[12b]$	$[12b]/[Ag^+]$	δ_{Ar} (ppm)	$\Delta\delta_{Ar}$ (ppm)	δ_{SCH_2} (ppm)	$\Delta\delta_{SCH_2}$ (ppm)	δ_{OCH_2} (ppm)	$\Delta\delta_{OCH_2}$ (ppm)
1	0.00	4.84×10^{-4}	0.00	0.00	**6.930**	0.000	**4.304**	0	**4.069**	0.000
2	2.41×10^{-4}	4.61×10^{-4}	0.52	1.91	6.964	0.034	4.353	0.049	4.083	0.014
3	3.17×10^{-4}	4.54×10^{-4}	0.70	1.43	6.977	0.047	4.369	0.065	4.088	0.018
4	3.90×10^{-4}	4.47×10^{-4}	0.87	1.15	6.982	0.052	4.380	0.076	4.089	0.019
5	4.61×10^{-4}	4.40×10^{-4}	1.05	0.96	6.988	0.058	4.392	0.088	4.092	0.023
6	6.29×10^{-4}	4.24×10^{-4}	1.48	0.67	7.002	0.072	4.414	0.110	4.095	0.026
7	7.85×10^{-4}	4.09×10^{-4}	1.92	0.52	7.017	0.087	4.432	0.128	4.099	0.029
8	9.31×10^{-4}	3.95×10^{-4}	2.35	0.42	7.021	0.091	4.446	0.142	4.102	0.032
9	1.07×10^{-3}	3.82×10^{-4}	2.79	0.36	7.029	**0.099**	4.457	**0.153**	4.103	**0.034**

Run #2:

Entry	$[Ag^+]$	[12b]	$[Ag^+]/[12b]$	$[12b]/[Ag^+]$	δ_{Ar} (ppm)	$\Delta\delta_{Ar}$ (ppm)	δ_{SCH_2} (ppm)	$\Delta\delta_{SCH_2}$ (ppm)	δ_{OCH_2} (ppm)	$\Delta\delta_{OCH_2}$ (ppm)
1	0.00	4.84×10^{-4}	0.00	0.00	**6.931**	0.000	**4.306**	0.000	**4.069**	0.000
2	2.41×10^{-4}	4.61×10^{-4}	0.52	1.91	6.963	0.032	4.355	0.049	4.084	0.015
3	3.17×10^{-4}	4.54×10^{-4}	0.70	1.43	6.976	0.045	4.369	0.063	4.088	0.019
4	3.90×10^{-4}	4.47×10^{-4}	0.87	1.15	6.985	0.054	4.382	0.076	4.092	0.023
5	4.61×10^{-4}	4.40×10^{-4}	1.05	0.96	6.990	0.059	4.393	0.087	4.092	0.023
6	6.286×10^{-4}	4.24×10^{-4}	1.48	0.67	7.003	0.072	4.416	0.110	4.097	0.027
7	7.85×10^{-4}	4.09×10^{-4}	1.92	0.52	7.015	0.084	4.433	0.127	4.102	0.033
8	9.31×10^{-4}	3.95×10^{-4}	2.35	0.42	7.026	0.095	4.446	0.140	4.105	0.036
9	1.07×10^{-3}	3.82×10^{-4}	2.79	0.36	7.031	**0.100**	4.456	**0.150**	4.108	**0.039**

Appendix 3 Chemical shift changes (Δδ) for the $–CH_2S-CH_2-$ protons on **12a** in 1:9 CD_3CN-$CDCl_3$ at 298 K *versus* added $HgCl_2$ solution (5.07×10^{-3} M) (Δδ are absolute values).

Run #1:

Entry #	$[Hg^{2+}]$ (mol/L)	$\frac{[Hg^{2+}]}{[OMe]}$	δ (ppm)	Δδ (ppm)
1	0.000E+00	0.0	4.301	0.000
2	1.644E-04	0.35	4.303	0.002
3	3.919E-04	0.87	4.305	0.004
4	5.661E-04	1.31	4.306	0.005
5	8.785E-04	2.18	4.309	0.008
6	1.390E-03	3.92	4.313	0.012
7	1.790E-03	5.67	4.316	0.015
8	2.113E-03	7.41	4.318	0.017
9	2.378E-03	9.16	4.321	0.020
10	2.600E-03	10.90	4.322	0.021

Run #2:

Entry #	$[Hg^{2+}]$ (mol/L)	$\frac{[Hg^{2+}]}{[OMe]}$	δ (ppm)	Δδ (ppm)
1	0.000E+00	0.0	4.301	0.000
2	1.644E-04	0.35	4.303	0.002
3	3.919E-04	0.87	4.305	0.004
4	5.661E-04	1.31	4.306	0.005
5	8.785E-04	2.18	4.309	0.008
6	1.390E-03	3.92	4.313	0.012
7	1.790E-03	5.67	4.315	0.014
8	2.113E-03	7.41	4.318	0.017
9	2.378E-03	9.16	4.320	0.019
10	2.600E-03	10.90	4.322	0.021

Appendix 4 Chemical shift changes (Δδ) for the $–CH_2S-CH_2-$ protons on **12b** in 1:9 CD_3CN-$CDCl_3$ at 298 K *versus* added $HgCl_2$ solution (5.07×10^{-3} M) (Δδ are absolute values).

Run #1:

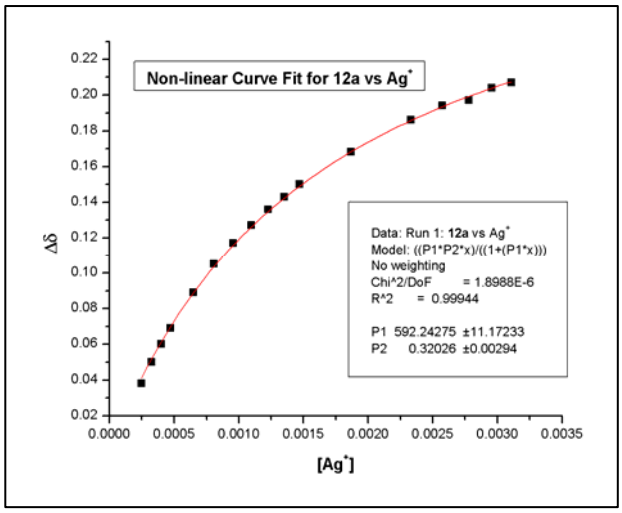
Entry #	$[Hg^{2+}]$ (mol/L)	[OEt] (mol/L)	$\frac{[Hg^{2+}]}{[OEt]}$	Δδ (ppm)
1	0.000E+00	4.838E-04	0.0	0.000
2	1.644E-04	4.682E-04	0.37	0.004
3	3.919E-04	4.466E-04	0.87	0.007
4	5.661E-04	4.301E-04	1.31	0.009
5	8.785E-04	4.004E-04	2.18	0.014
6	1.390E-03	3.519E-04	3.92	0.020
7	1.790E-03	3.138E-04	5.67	0.024
8	2.378E-03	2.580E-04	9.16	0.030
9	2.600E-03	2.370E-04	10.9	0.034

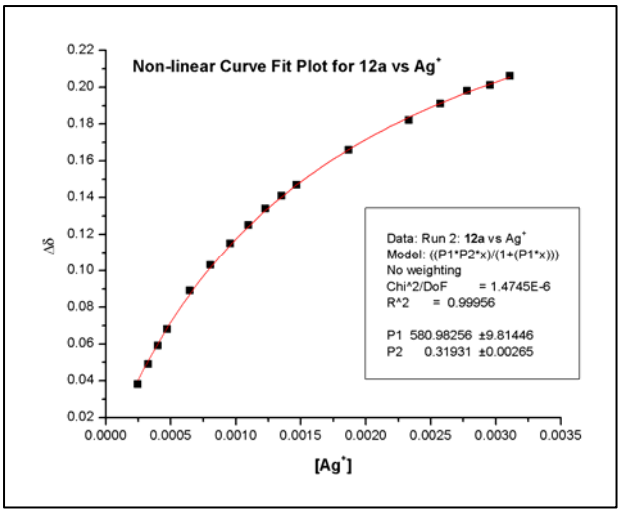
Run #2:

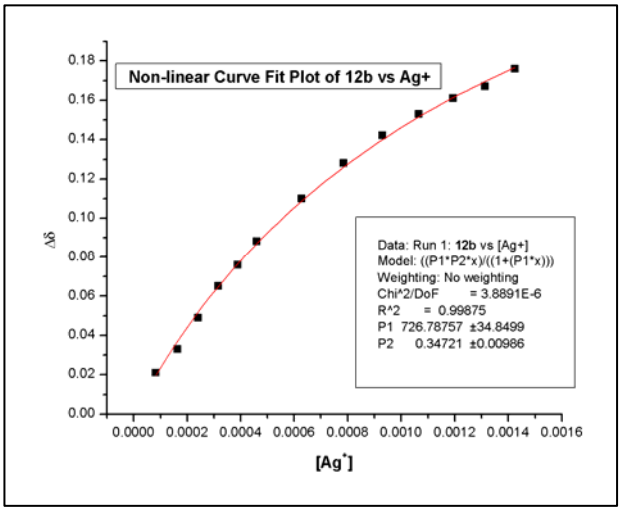
Entry #	$[Hg^{2+}]$ (mol/L)	[OEt] (mol/L)	$\frac{[Hg^{2+}]}{[OEt]}$	Δδ (ppm)
1	0.000E+00	4.838E-04	0.0	0.000
2	1.644E-04	4.682E-04	0.37	0.003
3	3.919E-04	4.466E-04	0.87	0.007
4	4.632E-04	4.398E-04	1.05	0.008
5	5.661E-04	4.301E-04	1.31	0.010
6	8.785E-04	4.004E-04	2.18	0.014
7	1.390E-03	3.519E-04	3.92	0.020
8	1.790E-03	3.138E-04	5.67	0.024
9	2.378E-03	2.580E-04	9.16	0.031
10	2.600E-03	2.370E-04	10.9	0.033

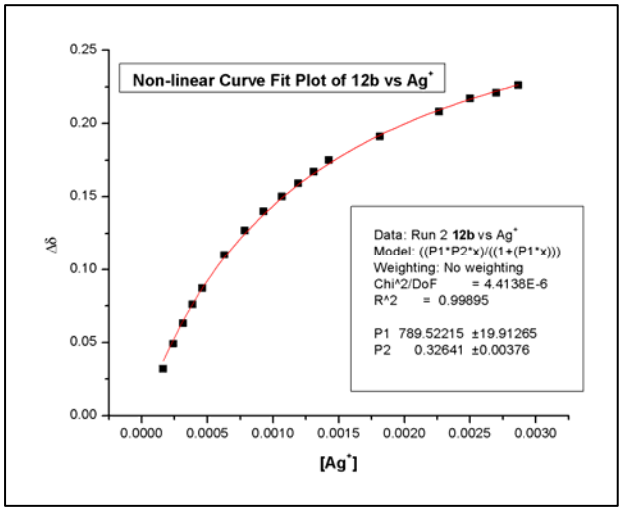
Appendix 5. Determinations of K_{assoc} for **12a:**Ag^+ (*top*) and for **12b:**Ag^+ (*bottom*) complexes in 1:9 CD_3CN-$CDCl_3$ at 298 K. AgO_2CCF_3 (5.22×10^{-3} M) solution was added as aliquots.

Left: Run 1; *Right* Run 2.









Appendix 6. Determination of K_{assoc} for **12a:**Hg^{2+} (*top*) and for **12b:**Hg^{2+} (*bottom*) complexes complexes in 1:9 CD_3CN-$CDCl_3$ at 298 K. $HgCl_2$ solutions (5.10 x 10^{-3} M) solution was added as aliquots.

Left: Run 1; *Right* Run 2.